Semiclassical analysis of a complex quartic Hamiltonian

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It is necessary to calculate the $\mathcal{C}$ operator for the non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian $H=\frac{1}{2}p^2+\frac{1}{2}\mu^2x^2-\lambda x^4$ in order to demonstrate that H defines a consistent unitary theory of quantum mechanics. However, the $\mathcal{C}$ operator cannot be obtained by using perturbative methods. Including a small imaginary cubic term gives the Hamiltonian $H=\frac{1}{2}p^2+\frac{1}{2}\mu^2x^2+igx^3-\lambda x^4$, whose $\mathcal{C}$ operator *can* be obtained perturbatively. In the semiclassical limit all terms in the perturbation series can be calculated in closed form and the perturbation series can be summed exactly. The result is a closed-form expression for $\mathcal{C}$ having a nontrivial dependence on the dynamical variables x and p and on the parameter λ.

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In this paper we consider a quantum system described by the Hamiltonian

$$H=\tfrac{1}{2}p^2+\tfrac{1}{2}\mu^2x^2+igx^3-\lambda x^4, \tag{1}$$

where g is real and nonzero and $\lambda\geq 0$. Note that the potential is complex and that when λ is positive the potential is unbounded below. This Hamiltonian is not Hermitian in the conventional sense, where Hermitian conjugation is defined as combined transpose and complex conjugate. Nevertheless, the eigenvalues E_n are all real, positive, and discrete. This is because H possesses an unbroken $\mathcal{PT}$ symmetry [1, 2], which means that H and its eigenstates $\psi_n(x)$ are invariant under space-time reflection. Here, $\mathcal{P}$ denotes the spatial reflection $p\to -p$ and $x\to -x$, and $\mathcal{T}$ denotes the time reversal $p\to -p$, $x\to x$, and $i\to -i$.

Many $\mathcal{PT}$-symmetric quantum-mechanical Hamiltonians have been studied in the recent literature [3, 4, 5, 6]. However, the Hamiltonian (1) is special because when $g\neq 0$ the boundary conditions on the eigenfunctions may be imposed on the real-x axis, as opposed to the interior of a wedge in the complex-x plane, as we will now show: The quantization condition satisfied by the eigenfunctions requires that $\psi_n(x)$ must vanish exponentially in a pair of wedges in the complex-x plane. These wedges are symmetrically placed with respect to the imaginary axis. The wedges have an angular opening of 60° and lie below the positive and negative real-x axes with the upper edges of the wedges lying on the real axis. Using a WKB approximation we can determine the asymptotic behavior of the eigenfunctions, and we find that the exponential decay of these wave functions is given by

$$\psi_n(x)\sim e^{\pm\sqrt{2\lambda}[ix^3/3+gx^2/(4\lambda)]}\quad(|x|\to\infty). \tag{2}$$

Thus, the wave functions are oscillatory on the positive and negative real-x axes when $g=0$. However, when g is nonzero the wave functions decay exponentially on the real axis as well as in the interiors of the wedges. Thus, taking $g\neq 0$ allows us to treat x as a real variable and to perform calculations on the real axis.

Being able to treat x as real is crucial. The domain of the eigenfunctions of $H=\frac{1}{2}p^2+\frac{1}{2}\mu^2x^2-\lambda x^4$ is the interior of a pair of 60°-wedges in the lower-half x-plane. Under space reflection $x\to -x$, this domain changes to the interior of a pair of 60°-wedges in the *upper*-half plane. Therefore, this Hamiltonian is not parity symmetric. However, when $g\neq 0$, the domain of the eigenfunctions of H in (1) includes the real-x axis. Thus, on the real-x axis, the parity operator $\mathcal{P}$ commutes with the $-x^4$ operator. This fact enables us to perform in this paper a perturbative calculation of $\mathcal{C}$. The $\mathcal{C}$ operator is needed to formulate a consistent quantum theory described by the non-Hermitian Hamiltonian (1).

To make sense of H in (1) we must identify the Hilbert space spanned by the eigenfunctions of H and then construct for this space an inner product that is positive definite. As shown in Ref. [2], an inner product defined with respect to $\mathcal{PT}$-conjugation leads to an indefinite metric of the type investigated earlier by Lee and Wick [7]. However, an inner product defined with respect to $\mathcal{CPT}$-conjugation leads to a positive definite metric, and hence positive probabilities [2, 8]. Here $\mathcal{C}$ denotes a linear operator analogous to the charge operator in particle physics. The operator $\mathcal{C}$ commutes with the Hamiltonian and its square is unity, so its eigenvalues are ± 1. Because $\mathcal{C}$ commutes with H, the time evolution of the theory is unitary; that is, the norm of a vector is preserved in time. Given the operator $\mathcal{C}$, we can construct the *positive* operator $e^Q=\mathcal{CP}$, which can, in turn, be used to construct by a similarity transformation an equivalent Hamiltonian $\tilde{H}\equiv e^{-Q/2}He^{Q/2}$. The Hamiltonian $\tilde{H}$ is Hermitian in the conventional sense [8], but it is a nonlocal function of the operators x and p.

Thus, the key step in formulating a consistent quantum theory based on the Hamiltonian (1) is to calculate the operator $\mathcal{C}$. When $\lambda=0$, one can use perturbation

theory to calculate the $\mathcal{C}$ operator as a series in powers of g [9]. However, for the more interesting case of a negative quartic interaction ($g = 0$, $\lambda > 0$), a perturbative calculation of $\mathcal{C}$ using conventional Poincaré asymptotics fails because to all orders in powers of λ the operator Q vanishes. Only nonperturbative techniques such as hyperasymptotics (asymptotics beyond all orders) [10] can be used to find the $\mathcal{C}$ operator for the Hamiltonian $H = \frac{1}{2}p^2 + \frac{1}{2}\mu^2 x^2 - \lambda x^4$.

The analysis in this paper is based on the observation that when $g \neq 0$, no matter how small, it is possible to use perturbative methods to calculate $\mathcal{C}$. Our perturbative calculation is organized as follows: First, we introduce the small positive parameter ϵ into the Hamiltonian (1) and consider

$$H = \tfrac{1}{2}p^2 + \tfrac{1}{2}\mu^2 x^2 + i\epsilon g x^3 - \epsilon^2 \lambda x^4. \qquad (3)$$

We seek a perturbation series in powers of ϵ. The coefficient of ϵ^n in this perturbation series is complicated, and thus our second step is to simplify the coefficient by making a semiclassical approximation in which we only retain leading order terms in Planck's constant $\hbar$. The result is a series in powers of g, and since we may take g arbitrarily small, our third step is to simplify the coefficient further by omitting all contributions from higher powers of g. The resulting infinite series can then be summed exactly and in closed form. Once the summation is performed, our fourth step is to set $\epsilon = 1$ to obtain the semiclassical approximation to $\mathcal{C}$ for the Hamiltonian (1). The Hamiltonian (3) was first considered by Banerjee [11]. In Ref. [11] the first seven terms in the perturbation expansion for the $\mathcal{C}$ operator are calculated (but not in the semiclassical regime).

We begin our analysis by recalling that the $\mathcal{C}$ operator can be expressed in the form $\mathcal{C} = e^Q\mathcal{P}$, where $Q = Q(x,p)$ is a function of the quantum dynamical variables x and p. In earlier work we showed that $\mathcal{C}$ can be determined by searching for an operator that satisfies the following three conditions [12]:

$$\text{(i) } [\mathcal{C}, \mathcal{PT}] = 0, \quad \text{(ii) } \mathcal{C}^2 = \mathbf{1}, \quad \text{(iii) } [H, \mathcal{C}] = 0. \qquad (4)$$

Substituting $\mathcal{C} = e^Q\mathcal{P}$ into (i), we obtain the condition $Q(x,p) = Q(-x,p)$, so $Q(x,p)$ is an even function of x. Substituting $\mathcal{C} = e^Q\mathcal{P}$ into (ii), we get $Q(x,p) = -Q(-x,-p)$. Since $Q(x,p)$ is even in x, it is odd in p. Finally, condition (iii) reads

$$[H, e^Q\mathcal{P}] = 0. \qquad (5)$$

Our objective is to determine the expression for the operator $Q(x,p)$, when H is given by (3). Let us write the Hamiltonian (3) in the form

$$H = H_0 + \epsilon H_1 + \epsilon^2 H_2, \qquad (6)$$

where H_0 is the Harmonic oscillator Hamiltonian, $H_1 = igx^3$, and $H_2 = -\lambda x^4$. The commutation relation (5) then implies

$$\begin{aligned} H_0 e^Q\mathcal{P} \;-\; e^Q\mathcal{P}H_0 + \epsilon\left(H_1 e^Q\mathcal{P} - e^Q\mathcal{P}H_1\right) \\ +\; \epsilon^2\left(H_2 e^Q\mathcal{P} - e^Q\mathcal{P}H_2\right) = 0. \end{aligned} \qquad (7)$$

Under parity we have

$$\mathcal{P}H_0\mathcal{P} = H_0, \;\; \mathcal{P}H_1\mathcal{P} = -H_1, \;\; \text{and } \mathcal{P}H_2\mathcal{P} \;=\; H_2. \qquad (8)$$

As noted above, H_2 for x real commutes with $\mathcal{P}$ because g is nonzero.

Substituting these relations into (7) and multiplying $\mathcal{P}$ from the right, we obtain

$$\begin{aligned} e^Q H_0 - H_0 e^Q \;&=\; \epsilon\left(e^Q H_1 + H_1 e^Q\right) \\ &\quad -\epsilon^2\left(e^Q H_2 - H_2 e^Q\right). \end{aligned} \qquad (9)$$

We then multiply by e^{-Q} on the left and get

$$\begin{aligned} H_0 - e^{-Q}H_0 e^Q \;&=\; \epsilon\left(H_1 + e^{-Q}H_1 e^Q\right) \\ &\quad -\epsilon^2\left(H_2 - e^{-Q}H_2 e^Q\right). \end{aligned} \qquad (10)$$

In order to analyze (10) we make use of the Campbell-Baker-Hausdorff relation

$$\begin{aligned} e^{-Q}He^Q \;&=\; H + [H,Q] + \tfrac{1}{2!}[[H,Q],Q] \\ &\quad + \tfrac{1}{3!}[[[H,Q],Q],Q] + \cdots \end{aligned} \qquad (11)$$

and the fact that Q can be expanded as a power series in ϵ:

$$Q = \epsilon Q_1 + \epsilon^3 Q_3 + \epsilon^5 Q_5 + \cdots. \qquad (12)$$

Substitution of (12) into the right side of (11) yields

$$\begin{aligned} e^{-Q}He^Q \;&=\; H + \epsilon[H,Q_1] + \tfrac{1}{2!}\epsilon^2[[H,Q],Q] \\ &\quad +\epsilon^3\left([H,Q_3] + \tfrac{1}{3!}[[[H,Q_1],Q_1],Q_1]\right) \\ &\quad +\epsilon^4\left(\tfrac{1}{2!}[[H,Q_3],Q_1] + \tfrac{1}{2!}[[H,Q_1],Q_3]\right. \\ &\qquad \left. +\tfrac{1}{4!}[[[[H,Q_1],Q_1],Q_1],Q_1]\right) \\ &\quad +\epsilon^5\left(\tfrac{1}{5!}[[[[[H,Q_1],Q_1],Q_1],Q_1],Q_1]\right. \\ &\qquad +\tfrac{1}{3!}[[[H,Q_1],Q_1],Q_3] + \tfrac{1}{3!}[[[H,Q_1],Q_3],Q_1] \\ &\qquad \left. +\tfrac{1}{3!}[[[H,Q_3],Q_1],Q_1] + [H,Q_5]\right) + \cdots. \end{aligned} \qquad (13)$$

Inserting the expansion (13) into (10) and equating coefficients of powers of ϵ, we obtain the following set of identities:

$$\begin{aligned} &[Q_1,H_0] = 2H_1, \\ &[Q_3,H_0] = \tfrac{1}{3!}[[[H_0,Q_1],Q_1],Q_1] + \tfrac{1}{2!}[[H_1,Q_1],Q_1] \\ &\quad +[H_2,Q_1], \\ &[Q_5,H_0] = \tfrac{1}{5!}[[[[[H_0,Q_1],Q_1],Q_1],Q_1],Q_1] \\ &\quad +\tfrac{1}{4!}[[[[H_1,Q_1],Q_1],Q_1],Q_1] \\ &\quad +\tfrac{1}{3!}[[[H_0,Q_1],Q_1],Q_3] + \tfrac{1}{3!}[[[H_0,Q_1],Q_3],Q_1] \\ &\quad +\tfrac{1}{3!}[[[H_0,Q_3],Q_1],Q_1] + \tfrac{1}{3!}[[[H_3,Q_1],Q_1],Q_1] \\ &\quad +\tfrac{1}{2!}[[H_1,Q_3],Q_1] + \tfrac{1}{2!}[[H_1,Q_1],Q_3] + [H_2,Q_3], \end{aligned} \qquad (14)$$

and so on. These identities correspond to the coefficients of ϵ, ϵ^3, and ϵ^5. The coefficients of the even powers of ϵ are redundant because they can be derived from the coefficients of the lower odd powers of ϵ. For example, the coefficient of ϵ^2 gives $[[H_0,Q_1],Q_1] = -2[H_1,Q_1]$, which follows from the first relation in (14).

We now perform a semiclassical approximation in which we only retain terms to leading order in $\hbar$. That is, we use the fact that each operator Q_i in (12) has a semiclassical expansion of the form

$$Q_i = \frac{1}{\hbar}Q_i^{(-1)} + Q_i^{(0)} + \hbar Q_i^{(1)} + \hbar^2 Q_i^{(2)} + \cdots, \qquad (15)$$

and discard all but the leading terms $Q_i^{(-1)}$ for $i = 1,3,5,\ldots$. Because we consider only the leading terms $Q_i^{(-1)}$, in what follows we omit the superscript and write Q_i for simplicity of notation.

We remark that in a semiclassical approximation, once a commutation relation is performed, we can regard x and p as classical variables and hence issues relating to operator ordering need not be considered. In this connection, the following relation applicable in semiclassical approximation is useful:

$$[p^a x^b, p^c x^d] = i\hbar(bc-ad)p^{a+c-1}x^{b+d-1}. \qquad (16)$$

This is a special case of the Poisson bracket relation

$$\{F(x,p),G(x,p)\} = i\left(\frac{\partial F}{\partial x}\frac{\partial G}{\partial p} - \frac{\partial F}{\partial x}\frac{\partial G}{\partial p}\right). \qquad (17)$$

Using the semiclassical commutation relation (16), we solve the first equation in (14) for Q_1 and obtain

$$Q_1 = -\frac{4g}{\mu^4\hbar}\Big[\tfrac{1}{3}p^3 + \tfrac{1}{2}\mu^2 p x^2\Big]. \qquad (18)$$

Substituting (18) into the second relation of (14) allows us to determine Q_3 as

$$\begin{aligned} Q_3 \;=\; & -\frac{4^2\lambda g}{\mu^8\hbar}\Big[\tfrac{2}{5}p^5 + \mu^2p^3x^2 + \tfrac{1}{2}\mu^4px^4\Big] \\ & + \frac{4^2 g^3}{\mu^{10}\hbar}\Big[\tfrac{8}{15}p^5 + \tfrac{5}{6}\mu^2p^3x^2 + \tfrac{1}{2}\mu^4px^4\Big]. \end{aligned} \qquad (19)$$

Similarly, substituting (18) and (19) into (14), we deduce that

$$\begin{aligned} Q_5 \;=\; & -\frac{4^3\lambda^2 g}{\mu^{12}\hbar}\Big[\tfrac{4}{7}p^7 + 2\ mu^2p^5x^2 + 2\mu^4p^3x^4 + \tfrac{1}{2}\mu^6px^6\Big] \\ & + \frac{4^3\lambda g^3}{\mu^{14}\hbar}\Big[\tfrac{16}{7}p^7 + 6\mu^2p^5x^2 + \tfrac{16}{3}\mu^4p^3x^4 + \tfrac{7}{4}\mu^6px^6\Big] \\ & - \frac{4^3 g^5}{\mu^{16}\hbar}\Big[\tfrac{5}{3}p^7 + \tfrac{17}{6}\mu^2p^5x^2 + \tfrac{8}{3}\mu^4p^3x^4 + \mu^6px^6\Big]. \end{aligned} \qquad (20)$$

Continuing in this manner, we can determine the perturbative expansion of Q explicitly. Observe, however, that Q_{2n+1} for each $n = 0,1,2,\ldots$ is an odd polynomial of g of degree $2n+1$. This follows from (14) if we notice that H_1 and hence Q_1 are proportional to g whereas H_0 and H_2 are independent of g. Because we assume that the Hamiltonian (1) has a weak cubic interaction, the value of the coupling g is small. Therefore, we may omit terms of order g^3 and higher from the expansion of Q. To first order in g the set of identities in (14) reduces to the following simpler set of relations:

$$\begin{aligned} \big[H_0,Q_1\big] &= -2H_1 \\ \big[H_0,Q_3\big] &= \big[Q_1,H_2\big] \\ \big[H_0,Q_5\big] &= \big[Q_3,H_2\big] \\ \big[H_0,Q_7\big] &= \big[Q_5,H_2\big] \\ &\vdots \end{aligned} \qquad (21)$$

From these relations we deduce that to first order in g, Q_7 is given by

$$\begin{aligned} Q_7 \;=\; & -\frac{4^4\lambda^3 g}{\mu^{16}\hbar}\Big[\tfrac{8}{9}p^9 + 4\ mu^2p^7x^2 + 6\mu^4p^5x^4 \\ & + \tfrac{10}{3}\mu^6p^3x^6 + \tfrac{1}{2}\mu^8px^8\Big], \end{aligned} \qquad (22)$$

and that to first order in g, Q_9 is given by

$$\begin{aligned} Q_9 \;=\; & -\frac{4^5\lambda^4 g}{\mu^{20}\hbar}\Big[\tfrac{16}{11}p^{11} + 8\mu^2p^9x^2 + 16\mu^4p^7x^4 \\ & + 14\mu^6p^5x^6 + 5\mu^8p^3x^8 + \tfrac{1}{2}\mu^{10}px^{10}\Big]. \end{aligned} \qquad (23)$$

By repeating this procedure and determining Q_{2n+1} for $n = 0,1,2,\ldots$, we deduce, in general, that

$$\begin{aligned} Q_{2n+1} \;=\; & -g\frac{2^{3n+2}\lambda^n}{\mu^{4n+4}\hbar}p \\ & \times\sum_{k=0}^{n+1}\frac{\mu^{2k}(2n-k+2)!}{2^k k!(2n-2k+3)!}x^{2k}p^{2n-2k+2}. \end{aligned} \qquad (24)$$

To determine the semiclassical expression for Q, we must sum the product $\epsilon^{2n+1}Q_{2n+1}$ in n. For convenience we define the variables

$$\alpha = \frac{\mu^2x^2}{2p^2} \quad \text{and} \quad \beta = \frac{8\epsilon^2\lambda p^2}{\mu^4}, \qquad (25)$$

and write

$$\epsilon^{2n+1}Q_{2n+1} = -\frac{4\epsilon g p^3}{\mu^4\hbar}\beta^n\sum_{k=0}^{n+1}\frac{(2n-k+2)!}{k!(2n-2k+3)!}\alpha^k. \quad (26)$$

By summing (26) in n and interchanging the orders of summation, we can express Q as

$$\begin{aligned} Q \;=\; & -\frac{4\epsilon g p^3}{\mu^4\hbar}\alpha\sum_{k=0}^{\infty}\frac{(\alpha\beta)^k}{(k+1)!}\sum_{n=0}^{\infty}\frac{(2n+k+1)!}{(2n+1)!}\beta^n \\ & -\frac{4\epsilon g p^3}{\mu^4\hbar}\sum_{n=0}^{\infty}\frac{1}{2n+3}\beta^n. \end{aligned} \qquad (27)$$

To determine the first sum in the right hand side of (27), we use the identity $(2n+k+1)! = \int_0^\infty dt\, t^{2n+k+1} e^{-t}$. After performing the resulting integral, we get

$$\alpha \sum_{k=0}^{\infty} \frac{(\alpha\beta)^k}{(k+1)!} \sum_{n=0}^{\infty} \frac{(2n+k+1)!}{(2n+1)!} \beta^n = \frac{1}{2\beta^{\frac{3}{2}}} \left[\ln \frac{1-\alpha\beta+\sqrt{\beta}}{1-\alpha\beta-\sqrt{\beta}} - \ln \frac{1+\sqrt{\beta}}{1-\sqrt{\beta}} \right]. \quad (28)$$

The summation on the left side of (28) converges to the right side provided that the inequality $\alpha\beta + \sqrt{\beta} < 1$ is satisfied. More explicitly, this inequality reads

$$p < -\epsilon\sqrt{2\lambda}\, x^2 + \frac{\mu^2}{2\epsilon\sqrt{2\lambda}}. \quad (29)$$

For $\epsilon \ll 1$, the summation on the left side of (28) converges essentially in the entirety of the semiclassical phase space. An analogous conclusion follows in the limit $\lambda \to 0$. For finite ϵ and λ, there is a parabolic region in the semiclassical phase space in which the operator Q converges. We believe that this region might be associated with the region in which the corresponding classical trajectories are confined, although we have not studied this question.

The second term on the right side of (27) gives

$$\sum_{n=0}^{\infty} \frac{\beta^n}{2n+3} = \frac{1}{\beta^{\frac{3}{2}}} \left(\frac{1}{2} \ln \frac{1+\sqrt{\beta}}{1-\sqrt{\beta}} - \sqrt{\beta} \right). \quad (30)$$

Note that the left side of (30) converges for $\beta < 1$, which holds automatically if (29) is satisfied.

Combining (28) and (30) and substituting (25), we finally deduce that to leading order in g the semiclassical expression for the operator Q associated with the Hamiltonian (3) is

$$\begin{aligned} Q &= -\frac{4\epsilon g p^3}{\mu^4 \hbar} \left(\frac{1}{2\beta^{\frac{3}{2}}} \ln \frac{1-\alpha\beta+\sqrt{\beta}}{1-\alpha\beta-\sqrt{\beta}} - \frac{1}{\beta} \right) \\ &= \frac{g\mu^2\sqrt{2}}{16\epsilon^2\lambda^{\frac{3}{2}}\hbar} \ln \frac{\mu^2 - 4\lambda\epsilon^2 x^2 - 2\epsilon\sqrt{2\lambda}\, p}{\mu^2 - 4\lambda\epsilon^2 x^2 + 2\epsilon\sqrt{2\lambda}\, p} - \frac{gp}{2\epsilon\lambda\hbar}. \end{aligned} \quad (31)$$

We have performed the summation explicitly, so we may set $\epsilon = 1$ in (31) to obtain the corresponding result for the Hamiltonian (1). This achieves our objective of finding the semiclassical approximation to the $\mathcal{C}$ operator for this Hamiltonian. Note that if we expand the right side of (31) for small λ and then take the limit $\lambda \to 0$, we recover (18). This is because, to first order in g, Q_1 is the only term that is not proportional to λ.

A complete analysis of the $\mathcal{C}$ operator for a $-\lambda x^4$ quantum-mechanical theory would be of immense importance because it could lead to an understanding of its $-\lambda\phi^4$ field-theoretic counterpart. This field theory is asymptotically free [13, 14, 15] and might well describe the Higgs sector in the standard model. Of course, the perturbative method used here does not apply directly to a pure quartic $-\lambda x^4$ theory, which is inherently nonperturbative; that is, we cannot set $g = 0$ to obtain the semiclassical expression for Q in the $-\lambda x^4$ theory. However, the work we have presented here is a first step towards our goal of obtaining a complete semiclassical and nonperturbative treatment of the $-\lambda x^4$ theory in quantum mechanics.

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